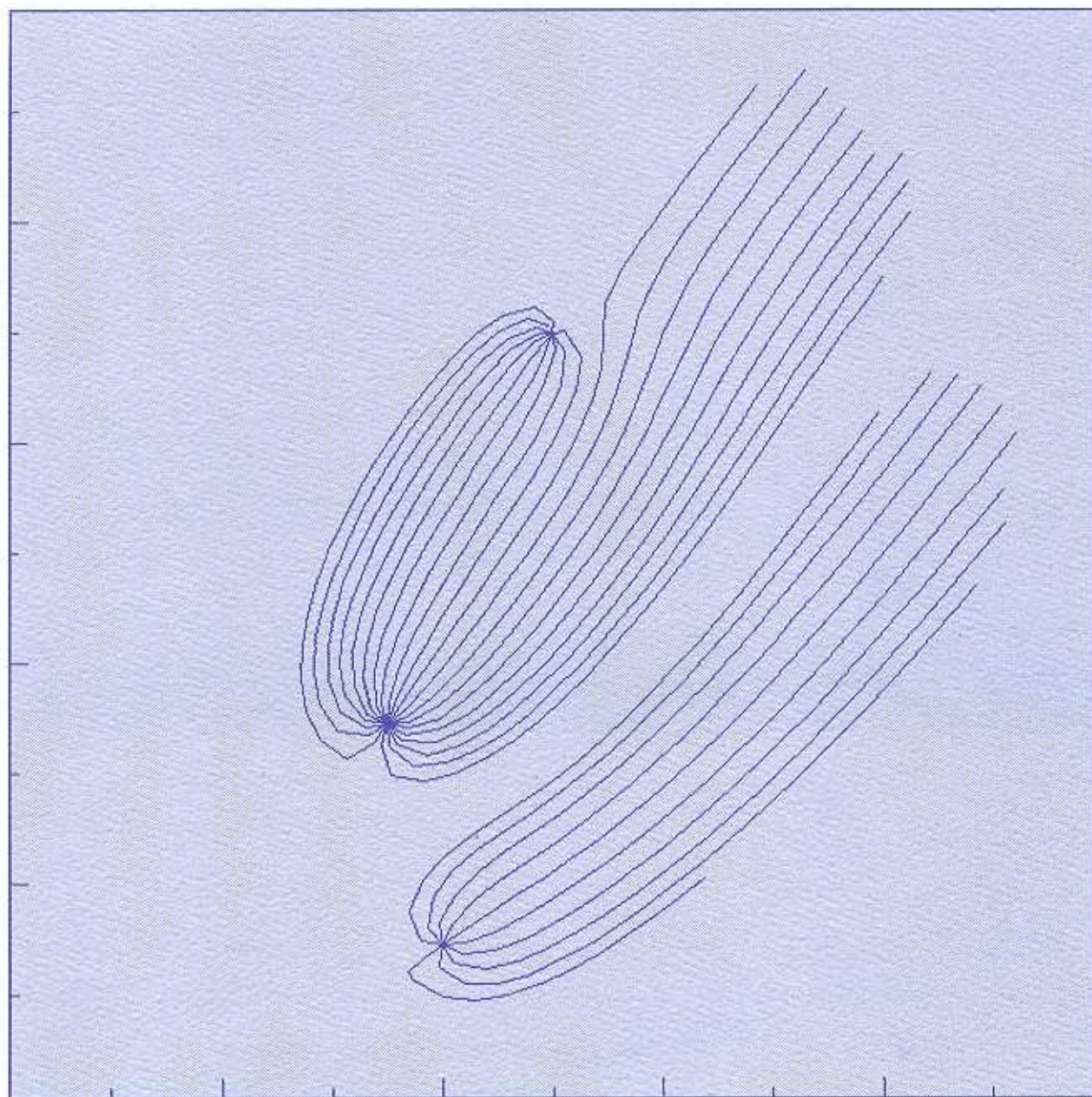


# Ground Water Modeling for Hydrogeologic Characterization

Guidance Manual for Ground Water Investigations



# GROUND WATER MODELING FOR HYDROGEOLOGIC CHARACTERIZATION

Guidance Manual for Ground Water Investigations

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## FOREWORD

The California Environmental Protection Agency (Cal/EPA) is charged with the responsibility of protecting the state's environment. Within Cal/EPA, the Department of Toxic Substances Control (DTSC) has the responsibility of managing the state's hazardous waste program to protect public health and the environment. The State Water Resources Control Board and the nine Regional Water Quality Control Boards (RWQCBs), also part of Cal/EPA, have the responsibility for coordination and control of water quality, including the protection of the beneficial uses of the waters of the state. Therefore, the RWQCBs work closely with DTSC in protecting the environment.

To aid in characterizing and remediating hazardous substance release sites, DTSC had established a technical guidance work group to oversee the development of guidance documents and recommended procedures for use by its staff, local governmental agencies, responsible parties and their contractors. The Geological Support Unit (GSU) within DTSC provides geologic assistance, training and guidance. This document was prepared by GSU staff in cooperation with the technical guidance work group and the RWQCBs. This document has been prepared to provide guidelines for the investigation, monitoring and remediation of hazardous substance release sites. It should be used in conjunction with the two-volume companion reference for hydrogeologic characterization activities:

*Guidelines for Hydrogeologic Characterization of Hazardous Substances Release Sites*  
*Volume 1: Field Investigation Manual*  
*Volume 2: Project Management Manual*

Please note that, within the document, the more commonly used terms, *hazardous waste site* and *toxic waste site*, are used synonymously with the term hazardous substance release site. However, it should be noted that any unauthorized release of a substance, hazardous or not, that degrades or threatens to degrade water quality may require corrective action to protect its beneficial use.

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## **1 INTRODUCTION**

### **1.1 Purpose**

This document provides guidelines for the application of ground water and contaminant transport models to the characterization of hazardous substance release sites. The purpose of this document is to aid in model selection, provide recommended quality assurance and quality control (QA/QC) procedures, and give a standardized approach to data presentation.

This guidance addresses the use of models for four primary purposes: 1) to better characterize the ground water regime at a site, 2) to predict contaminant transport, 3) to locate areas of potential environmental risk, and 4) to assess possible remediation or corrective action alternatives. This might include prediction of the future concentration of contaminants at a water supply well, design of a ground water extraction and injection system, aiding the design of monitoring well networks, and simulation of the effects of recharge and discharge on ground water flow and contaminant migration.

### **1.2 Application**

Mathematical models of ground water flow and contaminant transport are increasingly used to provide answers to hydrogeologic questions that arise at hazardous waste sites. The National Research Council (1989) studied the scientific and regulatory use of ground water models. As a result of this, they concluded in part, "regulatory agencies should provide detailed, consistent procedures for the proper development and application of models." The technical guidance in this document has been developed to ensure that 1) objectives are clearly defined for modeling studies, 2) ground water modeling studies meet well defined quality assurance criteria to ensure the highest possible accuracy, 3) reporting requirements are specified so that modeling studies can be independently reviewed, 4) selection of mathematical models is appropriate to the problem at hand, 5) the data set is adequate to approximate the real ground water system, and 6) the uncertainty intrinsic to the model is assessed and reported in order for decision makers to determine the value of the modeling effort.

Several criteria must be considered in ground water modeling. The U.S. Environmental Protection Agency (1988a) refers to these as objectives criteria, technical criteria, and implementation criteria. Objectives criteria deal with the purpose for modeling, whether for a screening study or a detailed site study. Technical criteria address the capability of a mathematical model to simulate the site specific processes of concern. Implementation criteria deal with the ease of obtaining, using, and demonstrating the acceptability of a model for a particular use. The proper selection and application of a model rely on many quality assurance procedures throughout the modeling process. Quality assurance for ground water modeling was discussed in detail by van der Heijde (1987) and Wilkinson and Runkle (1986).

Although the considerations above will determine the usefulness of a model for a particular site, it is the quality and quantity of site specific data that allow the model to simulate the real system, rather than just providing a generic model of a process. An adequate number of representative data points may allow the modeler to simulate site specific processes with a high degree of confidence. Modeling with limited data may enable the investigator to develop preliminary conclusions which may help guide an investigation in the early stages.

## Ground Water Modeling

While the computer code and mathematical procedures in some models is highly complex, and must be understood by the modeler to produce a useful simulation, the goal of modeling implied in this document is to provide an approximation of a site-specific situation. A qualified professional with a background in hydrogeology or ground water hydrology and experience in ground water modeling is best suited to determine whether a simulation is reasonable, and to present recommendations based on the modeling study.

The guidelines presented herein apply to modeling undertaken to characterize the flow of ground water and the transport of contaminants at a hazardous waste site, to predict the future concentrations and locations of contaminants in ground water for risk assessment, and to aid the design and application of remedial strategies for contaminated ground water. While few flow and transport problems can be modeled with absolute confidence, this technical guidance is presented to aid in the interpretation of modeling results to assist in decisions regarding hydrogeologic characterization, well placement, and ground water remediation.

This document is organized according to the process typically followed in the application of a numerical model (Figure 1). The guidelines presented here apply specifically to the use of numerical models. However, the requirements should also be met, to their applicable extent, when using analytical and semi-analytical models.

### 1.3 Limitations

Authorization of particular modeling procedures or computer programs is neither intended nor provided in this document. Blanket approval of a model is not possible. A model that is suitable for one purpose may not be suitable for another. Such approval would suppress innovation and the use of newer models.

This guidance document is not intended as an instructional reference for ground water modeling. Its purpose is to outline those elements that must be considered and reported in conducting a scientifically defensible modeling study. The guidance should be used by qualified professionals with backgrounds in hydrogeology and ground water modeling to ensure that modeling results and subsequent reporting are thorough and technically sound.

The guidance applies specifically to the modeling of ground water flow and contaminant transport in saturated porous media. Modeling of fracture flow, double porosity systems, multiple fluid phases, and other similar complex systems may be beyond the scope of this guidance. While models exist for these situations, the input parameters are often difficult or impossible to define adequately in the field. When such models are used, however, the guidance should be followed where applicable.

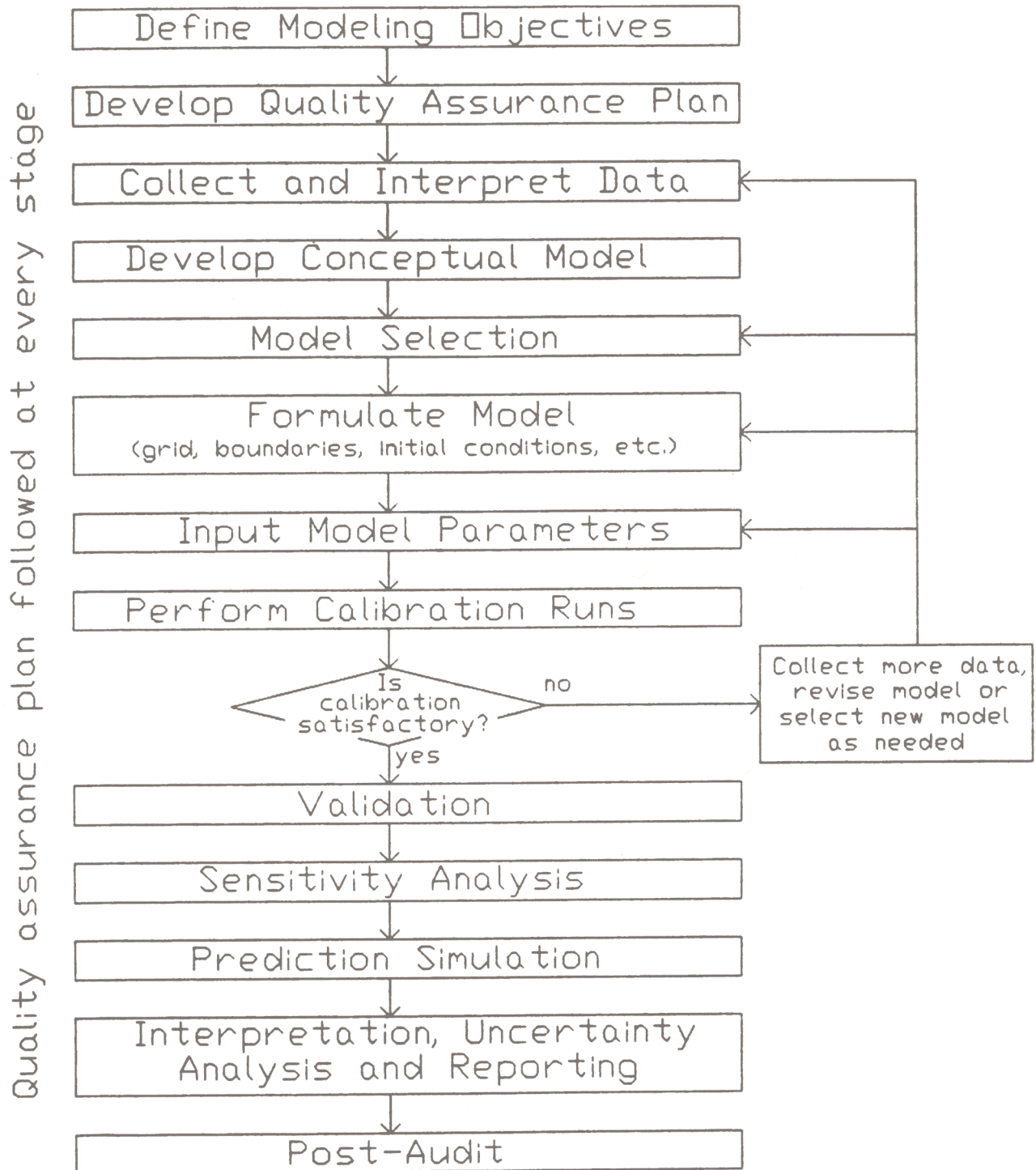


Figure 1. Flow diagram for the application of a numerical ground water model.

## **Ground Water Modeling**

Ground water modeling is a tool used to build on an existing sound understanding of site hydrogeologic conditions. This basic foundation must be developed through a thorough hydrogeologic site characterization. A ground water model cannot be used as a substitute for data collection in the field (National Research Council, 1989). Characterization of the hydrogeology of a site or facility is required by both federal and state regulations. Comprehensive hydrogeologic characterization is essential for undertaking hydrogeologic modeling to be used in decision making.

This document does not supersede existing statutes and regulations. Federal, state and local regulations, statutes, and ordinances must be identified when required by law, and site characterization activities must be performed in accordance with the most stringent of these requirements where applicable, relevant and appropriate.

## **2 MODELING OBJECTIVES**

Ground water models are commonly used to:

- Identify data gaps during hydrogeologic characterization,
- Aid in the design of a monitoring well network capable of detecting a release from a waste disposal facility,
- Determine the potential impacts of contaminated ground water on nearby wells or surface water bodies, and
- Aid in selection and design of remedial actions to control, or remove and treat, contaminated ground water.

The level of detail required to meet these objectives will depend on many factors, including the regulatory requirements to be served by the modeling study, the potential risk to public health or the environment from making a wrong decision based on model results, the complexity of site hydrogeology, and economic constraints. For example, the level of detail necessary to provide a conceptual understanding of ground water flow at a site may be much lower than that necessary to assess exposure of a nearby population to ground water contamination or to trigger regulatory action. Modeling objectives must be stated clearly and fully at the beginning of the project and in the professional report.

U.S. EPA (1988a) differentiates between using models for screening studies and detailed studies. Screening studies are undertaken to make general comparisons of several sites or several scenarios at a single site. Detailed or site-specific studies are undertaken to make detailed assessments of the environmental impact or performance of a site or facility. The National Research Council (1989) stated emphatically that screening or generic models can never be used as a replacement for site-specific models.

## **3 QUALITY ASSURANCE PROGRAMS**

Quality assurance is a major part of most investigation activities at hazardous waste sites. Collection and analysis of quality control samples may entail 10-25% of the soil or ground water sampling budget of projects. Many authors have recognized the need for, and the common lack of, quality assurance in both the development and application of ground water models (van der Heijde, 1987). Unfortunately, quality assurance for ground water modeling has been ignored in many cases, or considered only near or at the end of a project.

Development of a quality assurance plan at the beginning of a modeling study will help to ensure more reliable results.

Quality assurance considerations have been identified by several authors (National Research Council, 1990; van der Heijde, et al, 1988). The following should be included in a quality assurance plan:

- Protocols for field data collection, verification, and processing,
- Narrative and graphical presentation of a conceptual model, including description of processes to be considered,
- Criteria for model selection,
- Documentation and retesting when changes are made to a model code,
- Protocols to be followed in model formulation,
- Protocols to be followed in model calibration, limits on parameter adjustments, identification of calibration goals,
- Protocols for sensitivity analysis,
- Procedures for analysis of error,
- Level of information to be included in computer output,
- Applicability of the specific modeling program and mathematical formulas,
- Assumptions made and their potential influence on model output,
- Establishment of record keeping procedures to document the model application process, and
- Format for presentation of results.

## **4 SITE CHARACTERIZATION AND DATA COLLECTION**

To provide an approximation of site specific ground water flow and contaminant transport conditions, data used to construct the simulation and calibrate the model must be from site specific measurements. Measurements of parameters must be taken in a manner that ensures they are representative of field conditions, and the density of measurements must accurately depict the distribution of aquifer properties, ground water potential head, contaminant concentrations, and other parameters. Appropriate quality control measures must be followed in the collection of data to be used in modeling.

Ground water modeling data needs should be considered, along with other factors, when designing field programs for data collection. Modelers should participate in the collection of field data or work closely with field personnel. At a minimum, data used in ground water

modeling should be checked for accuracy, completeness, and representativeness. The uncertainty in field data will be a major factor in the uncertainty of model results.

To mathematically simulate the behavior of ground water and contaminants at a site, it is first necessary that the modeler have a detailed conceptual understanding of the site hydrogeology. This understanding should be developed using appropriate field and data analysis methods. Development of a conceptual model should include the construction of ground water contour maps and flow nets, or other methods to characterize the nature of ground water flow. The need to collect and properly interpret field measurements cannot be stressed strongly enough. McLaughlin and Johnson (1987) analyzed three modeling studies that used the same model and data set. Results varied widely, primarily because of differences in the interpretation of field conditions. Modeling studies are often conducted by personnel that are not familiar with site conditions, or have not even been to the site. It is highly desirable that the person or team conducting modeling also be familiar with the field conditions at the site.

## 5 MODEL SELECTION CRITERIA

The rationale for selecting a particular model should be presented for review. The model should have the capability of simulating the important processes identified in the conceptual model, as well as the dimensions, boundary conditions, and heterogeneity of the conceptual model. These technical criteria will be discussed in detail below. Compilations of the characteristics of available models have been published (U.S. EPA, 1988a) to aid in model selection. The staff and publications of the International Ground Water Modeling Center (IGWMC) can also be a valuable resource in the model selection process.

A generic model should not be selected to answer site specific questions. Even a generic model used to simulate a worst case scenario may be inappropriate because it may 1) be an arbitrary distortion of the remedial selection process, 2) reduce protection of the public health by mis-allocating finite cleanup resources, and 3) result in the imposition of substantial costs with no commensurate environmental or public health benefit (National Research Council, 1989).

### 5.1 Governing Equations/Process Equations

The model selected must be capable of solving the process equations for all processes that are found, through proper site characterization, to be important to the movement of ground water and contaminants at the site. These processes fall into the broad categories of transport and transformation processes.

All modeling must include the simulation of the advective flow of ground water at the site. Although other transport and transformation processes may be simulated, the model of the transport of contaminants can achieve no better accuracy than the ground water flow simulation, since advective flow is normally the major contaminant transport process. Flow and contaminant transport models may be separate or linked, but in either case flow will be solved by either a potential head or streamline derivation of the governing equations of ground water flow.

Other transport processes that may be considered are mechanical dispersion and diffusion. These processes are often lumped into a single dispersion parameter for modeling purposes. This is reasonable in most cases because diffusion is usually small in comparison to mechanical dispersion (Mercer and Faust, 1980b). The effects of varying fluid density, caused by high concentrations of contaminants, may also drive fluid transport.

Transformation processes generally reduce the concentration of a contaminant of interest, but may increase the concentration of another species. Transformation processes, such as biodegradation, hydrolysis and oxidation-reduction reactions change the physical or chemical state of a contaminant. Volatilization may reduce a contaminant concentration, but may also serve to cause transport in the gaseous phase.

Modeling of contaminant transport should include consideration of all transport and transformation processes that are significant at the specific site. Technical justification should be provided in the professional report for excluding or combining any transport or transformation processes.

While it is important to select a model that is capable of simulating all of the important processes occurring in the subsurface, selection of a model that is too complex may also lead to problems. An overly complicated model may require input parameters that cannot be accurately obtained from field measurements, leading to uncertainty in results, and overly complicated models may lead to excessive setup and operation costs (National Research Council, 1989).

### 5.2 Model Spatial Configuration.

The model selected must have the capability to represent the configuration of the volume of interest. This includes not only the geometry and dimensions of the ground water system to be simulated, but the following aspects that were identified in the conceptual model:

- Unconfined, confined, or semi-confined aquifers and the ranges of seasonal ground water elevation change
- Initial and boundary conditions
- Sources and sinks of water and their quantitative effects
- Sources of contaminants
- Physical and chemical characteristics of contaminants.

All real ground water systems, contaminant sources, and other features discussed are three-dimensional. A one- or two-dimensional model may simulate a ground water system, but only when the distribution of values for parameters in a particular dimension can be integrated into a single value. An example is an aquifer in which flow velocities and contaminant concentrations are equally distributed in the vertical direction. Lack of three-dimensional data is not a justification for performing a two-dimensional simulation. When a one- or two-dimensional model is applied, a

detailed technical justification should be presented for simulating the system in less than three dimensions.

### 5.3 Temporal Simulation

The model selected should have the capability of simulating the temporal state of the ground water regime. Steady state models provide average, long-term results. Transient models should be used when the ground water regime varies over time. Pumping, recharge, contaminant releases, and other stresses may vary, and this variability should be simulated as necessary to meet the modeling objectives.

### 5.4 Porous Media Properties.

Many properties of geologic materials have an effect on ground water flow and contaminant transport. The most important property controlling flow is the hydraulic conductivity. Properties such as effective porosity and percentage of clay minerals and organic materials control the rate of movement of contaminants.

In natural systems the properties of a porous medium usually vary in three dimensions. Variability may take the form of heterogeneity, anisotropy or both. Heterogeneity is the variation of a property of a material from point to point. Anisotropy is the variation of a property depending on the direction in which it is measured. As an example, stream-deposited sediments may be very heterogeneous, ranging from coarse stream gravels with high hydraulic conductivity to fine overbank deposits of much lower hydraulic conductivity. In addition, alluvial deposits often exhibit anisotropic hydraulic conductivity, due to non-random orientation of particles deposited by flowing water. Hydraulic conductivity in the original direction of streamflow is greater than in the cross stream direction, and much greater than that in the vertical direction.

To approximate the behavior of a ground water system, a model must be capable of simulating the heterogeneity and anisotropy of the system as identified in the conceptual model. Lack of adequate data is not an acceptable reason for treating a ground water system as homogeneous or isotropic. A detailed technical justification should be provided in the professional report for treating the ground water system as homogeneous or isotropic.

### 5.5 Fluid Properties

In their simplest form, the equations governing ground water flow apply only to water of constant density. Some variation in density caused by varying concentrations of solutes may be insignificant and introduce little error. Large variations in temperature or concentration of solutes, however, may cause density variations that must be considered to construct an accurate model. These cases require a more complicated formulation of the equations governing ground water flow, and a model that solves these equations. The modeling of multiple fluid phases, such as air and water or immiscible organic chemicals and water, is beyond the scope of these guidelines, but they should be addressed to the extent applicable.

## **6 MODEL DOCUMENTATION**

Whether it is a public domain model, a commercially available model, or a model developed for a specific project, model documentation must be provided in the professional report. Documentation should discuss the process equations solved by the model, the assumptions and limitations inherent in the model solution, the numerical or analytical solution techniques employed, and discussion of the structure of the model code. Any modifications made to the model for the particular study should be discussed. In addition, peer review by independent, qualified modelers of the conceptual and mathematical elements of the model should be demonstrated, and examples of previous uses of the model should be presented. The documentation may simply be referenced to readily available public domain sources, but in other cases a reproduction of the model documentation may be required as an appendix to the professional report.

Though models developed for a specific study may be used, extensive documentation must be provided. The time necessary to develop this documentation and go through a peer review process may prove to be infeasible. With numerous models of varying capabilities available, it is expected that newly developed models will not commonly be used to satisfy these guidelines. Unique algorithms that are not described in the model documentation, or which may be considered trade secrets, should not be used in models because the appropriateness of the model cannot be independently verified. Proprietary models may be used, but complete documentation, including sample runs, must be provided. These recommendations are in no way meant to discourage the use of proprietary models or the development of new models.

## **7 MODEL IMPLEMENTATION**

Once an acceptable model has been selected, implementation includes the steps of obtaining the model and documentation, installing the model on the computer system to be used, and verifying the numerical model by comparing results to analytical solutions.

### **7.1 Model Installation**

When using a commercially available or public domain computer model, it is important to install the model properly on a system similar to that used or recommended in the model documentation or user's manual. If a model is altered to run on another system, modifications should be discussed in the professional report.

To ensure that installation has been properly completed, one must recreate example problems given in the documentation.

### **7.2 Model Verification**

Verification is the process of checking the accuracy of the algorithms used to solve the necessary governing equations (van der Heijde, 1987), thereby demonstrating that the model actually approximates the process equations for which it is being applied. This can be accomplished by solving a problem with the model and comparing the results to those obtained from an analytical solution or another numerical model that has been verified. The problems solved for verification should be similar to the problem to which the model will be applied. If a model has been verified in the literature or user's manual, evidence of this should be presented. The

publication of a model or its availability for sale does not provide verification. The results of verification should be presented in the professional report.

## 8 SIMULATION

The following guidance applies to the process of using the model, properly selected and implemented, to simulate site specific conditions. The process of model application to specific case studies is presented in detail by Anderson and Woessner (1992).

### 8.1 Boundaries

In this stage of model setup, it is desirable to represent the physical boundaries that were identified in the conceptual model. Franke, Reilly and Bennett (1987) discussed the proper definition of boundary and initial conditions. Boundary conditions may be of three types: specified head or Dirichlet boundaries (includes constant head boundaries), specified flux or Neumann boundaries (includes no flow boundaries), and mixed or Cauchy boundaries. If the specification of physical boundaries is infeasible, or if the exact location of physical boundaries cannot be defined, non-physical boundaries may be defined for modeling purposes. These boundaries should be chosen so their location has no significant effect on model results in the area of interest. The effect the boundaries have on the model results can be determined by moving the boundaries and comparing results in an interior portion of the model. This testing method can also be used when physical boundaries cannot be located exactly, such as the subsurface trace of a fault.

### 8.2 Network Design

Most numerical methods require the specification of a network of nodes or cells within the model boundaries. Proper design of this network is important to accurately represent boundaries, sources and sinks, and other features. Good network design also helps ensure the accuracy of results in areas of greatest interest, by reducing the node spacing in these areas, thereby increasing resolution. Finite element models offer greater flexibility of grid design than many other solution techniques.

Mercer and Faust (1980c) list the following guidelines for grid design:

- Locate "well" nodes near the physical location of a pumping well or near the center of the well field.
- Locate boundaries accurately. For distant boundaries, the grid may be expanded, but avoid large spacings next to small ones.
- Nodes should be placed closer together in areas where there are large spatial changes in transmissivity or hydraulic head.
- Align axes of the grid with the major directions of anisotropy.

The node or cell network for a simulation should be sufficient to accurately reflect boundary conditions and geometry, and to provide necessary detail in areas of

greatest interest. The rationale for network design should be discussed, and the design depicted graphically, in the professional report.

### **8.3 Initial Input Parameters**

The model must generally have values specified initially for all parameters. The parameters may include head distribution, hydraulic conductivity, transmissivity, storativity, dispersivity, recharge, pumping, injection, etc., depending on the type of model. The proper specification of initial conditions is critical to transient models. The values of these parameters should be obtained from field measurements at the site. Geostatistical or other methods may be necessary to interpolate the necessary input data set from the field measured data.

The values of all input parameters for each model node or cell should be specified in tabular or graphical form. The source of the values for each parameter should be specified. Any methods used to process field-measured data to obtain model input should be specified and discussed in the technical report.

### **8.4 Calibration**

Calibration is the iterative process of adjusting the parameters in the model, such as hydraulic conductivity, transmissivity and dispersivity, so the model adequately approximates the real ground water system. This is accomplished by comparing the model results to a set of field observations. The calibration data set should include measurements over the lateral and vertical extent of the model area. For a flow model this data will often consist of water level measurements from monitoring wells and piezometers. Calibration to observed hydraulic head gradients, rather than head measurements is more difficult, but may be more representative for problems dealing with flow velocity and transport. Contaminant concentrations measured in ground water samples will be used to calibrate a contaminant transport model. The calibration data set, including all data point locations (monitoring wells, etc.), and the values of potential head or contaminant concentration that are being used for calibration, should be specified in the professional report.

Calibration is evaluated by analyzing the residuals, or differences between observed and simulated values, at specific locations. Calibration may be conducted by trial and error, changing the values of parameters until a good correlation is obtained between observed behavior of the ground water regime and the model results. Calibration goals should be stated in the quality assurance plan. Linear programming or other optimization techniques may also be used to calibrate the model (Cooley, 1977; Carrera and Neuman, 1986). The method used for calibration, and the number of runs necessary to achieve calibration should be specified in the professional report. Calibration should proceed by first changing those parameters with the lowest level of accuracy, and then fine-tuning the simulation by adjusting other parameters. Parameters should be adjusted within a reasonable, limited range relative to field measured values. Criteria for an acceptable calibration should be defined in an appropriate quality assurance plan. The rationale and assumptions used to adjust hydrogeologic parameters during calibration should be presented in the professional report.

The comparison of model results and observed values must be presented in tabular and graphical formats. Potential head measurements or contaminant concentrations should be presented in the form of contour maps and cross sections of observed and simulated values. The general shape of the potentiometric surface should be similar, including mounds, depressions and general flow directions. An x-y scatter plot of observed versus simulated heads will show the magnitude and any trends in residuals. A mass balance of water flow and contaminant mass (for transport models) should be presented for the calibrated model.

### **8.5 Final Input Parameters**

The calibration process consists of changing the initial input parameters, to simulate a data set of field observations. This results in parameters in the model not having their field measured values. The modeler must demonstrate that parameter values still lie within a reasonable range (i.e., that the model is still physically realistic for site conditions).

The final values for all parameters used in the calibrated model should be listed in tabular form, or presented in graphical form, for each cell or node. These should be compared with the initial input parameters, and checked to ensure that they are physically reasonable for the ground water regime.

### **8.6 Validation**

The calibration process, adjusting parameters in the model until the simulation closely matches observed values, creates a non-unique solution. Many different combinations of parameters may give results that meet the calibration criteria; each combination may fit better in some areas of the site and worse in others. For this reason, calibration alone cannot be accepted as verification of a model's accuracy. Freyberg (1988) showed that a good model calibration does not necessarily lead to good predictive capabilities. Therefore, the model must be validated, if possible, to further ensure that it accurately represents the ground water regime.

Validation is the process of comparing the calibrated model to another, independent, data set for the ground water regime. This should be another historical period with different stresses, which will demonstrate the predictive capability of the calibrated site model. The use of two data sets, if they corroborate each other, adds a degree of confidence. The quality of validation testing depends on the degree to which the site simulation is "stressed beyond" the calibration data on which it is based (van der Heijde, 1987). If the calibrated model truly approximates the physical behavior of the ground water regime, it should provide a reasonably good simulation of the validation data set.

Failure of the model to approximate the validation data set indicates the need for better calibration, or that a significant process has been ignored or improperly defined. At this stage, the model may be further calibrated with the validation data set and then checked against the calibration data set. An iterative process may be carried out until the model can simulate both data sets. If this cannot be achieved, it may be necessary to redefine the conceptual model.

The validation data set, including the measurement locations, monitoring wells, etc., and the values of potential head or contaminant concentration, which are being used for validation, should be specified in the professional report. The model results and observed values used for validation should be presented in tabular and graphical form as discussed in the calibration section above.

### 8.7 Sensitivity Analysis

Sensitivity analysis is the process of characterizing the effects of changes in parameters or boundary conditions on the behavior of the calibrated model. Sensitivity analysis can be performed both before and after model calibration. Before calibration, sensitivity analysis can identify the primary factors to be considered during calibration. When performed after calibration, sensitivity analysis helps to define the effect of parameters on model results.

Sensitivity analysis is conducted by altering model parameters and boundary conditions within reasonable ranges and observing changes in simulation results. If a small change in a parameter produces a large change in model results, the model is sensitive to that parameter. Sensitive parameters should be characterized by good field data to reduce uncertainty in model results. It was noted by van der Heijde (1987) that when models are coupled, such as coupled flow and transport models, study of the propagation of errors and the increasing uncertainty must be a part of sensitivity analysis. U.S. EPA gives an example of a sensitivity analysis for the ground water model of the San Gabriel Basin (U.S. EPA, 1988b).

### 8.8 Prediction

When the model has been calibrated and validated it may be used to simulate the future movement of ground water and contaminants or to simulate the response of the ground water system to various remedial action scenarios. Conditions that are vastly different from the calibration and validation conditions, such as high pumping rates or drawdowns, may invalidate the model as a representation of the physical system. The response of the model to various prediction scenarios should be presented in both narrative and graphical forms.

## 9 ERROR ANALYSIS

There are many sources of error in ground water modeling. These error sources fall into four major categories:

- Conceptual errors are those involving the application of an inappropriate model to a field situation. To avoid conceptual errors, a valid conceptual model of the ground water regime must be developed, and all the assumptions and limitations of the mathematical model must be understood. Following the guidance for conceptual models and model selection will guard against conceptual errors.
- Data errors are those resulting from the use of non-representative data describing field conditions. All data collected and used in modeling must be of high quality.

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- Truncation error occurs when differential equations are replaced by a set of algebraic equations (Mercer and Faust, 1980a). The amount of truncation error can be determined by repeating model runs with smaller node spacings and time steps. Significant changes in model results indicate truncation error. Decreasing time steps and node spacings should be used until truncation error is negligible.
- Round-off error also occurs in the numerical solution, due to finite accuracy of computer calculations. In a well coded computer model, this is generally the least important source of error.

All potential sources of error in the simulations should be evaluated and discussed in the professional report. The magnitude of all errors should be estimated.

## 10 POST-AUDIT

This guidance covers the use of models to predict ground water behavior in the future. Monitoring will often occur after the modeling study is completed. Unfortunately, only rarely is the continued monitoring used to check, and then improve, the ground water simulation. Konikow (1986) stated that if a model is to be used for prediction, it should be periodically post-audited, or re-calibrated, to incorporate new information. At the time of completion of the prediction phase of a modeling study, a plan should be made to check the model results both in time and in space. This may be accomplished by continuing monitoring and by the installation of additional wells or piezometers.

Konikow (1986) and Lewis and Goldstein (1982) have compared observed data from a period following a modeling effort with the predicted results. Model predictions have been shown to be only moderately successful in many cases. These results stress the need for a post-audit to improve the simulation or the resulting remedial action.

## 11 INTERPRETATION AND REPORTING OF RESULTS

The professional report describing the modeling study should present information on all of the elements discussed above in a manner that allows independent review, and allows the results to be reproduced from the information submitted. A narrative description and interpretation of the process and results of the modeling study should be presented in the professional report. The range of possible values for the processes of interest, and the level of confidence in the modeling results should be discussed. All modeling results should be critically evaluated to ensure that they are physically reasonable. The manner in which the results should be used to make decisions regarding the site should be presented. The results of computer models can appear more accurate or certain than they really are. To counteract this tendency, the National Research Council (1989) concluded, "All models must state quantitatively, to the extent possible, and if not quantitatively, then qualitatively, the degree and direction of uncertainty in the model results and the time frame over which the model's prediction can be considered acceptable." In addition, the uncertainty should be stressed whenever the model results are discussed. Only with this information can a decision maker give modeling results the proper weight when considering them along with other information.

Interpretations of model results should be reported in a clear and concise manner. The questions posed in the modeling objectives should be fully addressed, or additional study recommended. Confirmation that the QA plan was followed throughout the modeling study should be presented.

### REFERENCES

- Anderson, M.P. and W.W. Woessner. 1992. Applied groundwater modeling: simulation of flow and advective transport. Academic Press. Orlando, Florida.
- Boonstra, J. and N.A. deRidder. 1981. Numerical modelling of groundwater basins. International Institute for Land Reclamation and Improvement, Publication no. 29, 226 p.
- California Department of Health Services. 1986. California site mitigation decision tree manual. Chapter 3. Toxic Substances Control Program.
- Carrera, J. and S.P. Neuman. 1986. Estimation of aquifer parameters under transient and steady state conditions, 1. Maximum likelihood method incorporating prior information. *Water Resources Research*, v. 22, n. 2, p. 199-210.
- Cooley, R.L. 1977. A method for estimating and assessing reliability for models of steady-state ground-water flow, 1. Theory and numerical properties. *Water Resources Research*, v.13, p. 318-324.
- Franke, O.L., T.E. Reilly and G.D. Bennett. 1987. Definition of boundary and initial conditions in the analysis of saturated ground-water flow systems - an introduction. U.S. Geological Survey, Techniques of Water Resources Investigations, Book 3, Chapter B5., 15 p.
- Freyberg, D.L.. 1988. An exercise in ground-water model calibration and prediction. *Ground Water*, v. 26, n. 3, p. 350-360.
- Konikow, L.F.. 1986. Predictive accuracy of a ground-water model - lessons from a post-audit. *Ground Water*, v. 24, n.2, p. 173-184.
- Lewis, B.D. and F.J. Goldstein. 1982. Evaluation of a predictive ground-water solute-transport model at the Idaho National Engineering Laboratory. Idaho. U.S. Geological Survey Water Resources Investigation Report 82-25.
- McLaughlin, D. and W.K. Johnson. 1987. Comparison of three groundwater modeling studies. *ASCE Journal of Water Resources Planning and Management*. v. 113, n. 3, p 405-421.
- Mercer, J.W. and C.R. Faust. 1980a. Ground-water modeling: An overview. *Ground Water*, v.18, n.2, p. 108-115.
- Mercer, J.W. and C.R. Faust. 1980b. Ground-water modeling: Mathematical models. *Ground Water*, v.18, n.3, p. 212-227.
- Mercer, J.W. and C.R. Faust. 1980c. Ground-water modeling: Numerical models. *Ground Water*, v.18, n.4, p. 395-409.
- National Research Council. 1989. Ground water models: Scientific and regulatory applications. National Academy Press, Washington, D.C.
- United States Environmental Protection Agency (U.S. EPA). 1985. Characterization of hazardous waste sites - A methods manual, Volume 1 - Site investigations. Environmental Monitoring Systems Laboratory, EPA 600/4-84/075.
- U. S. EPA. 1986. RCRA ground water monitoring technical enforcement guidance document. OSWER-9950.1.

## Ground Water Modeling

U. S. EPA. 1987a. A compendium of Superfund field operations methods. EPA/540/P-87/001 (OSWER Directive 9355.0-14).

U. S. EPA. 1987b. The use of models in managing ground-water protection programs. EPA/600/8-87/003.

U. S. EPA. 1988a. Selection criteria for mathematical models used in exposure assessments: Ground-water models. EPA/600/8-88/075.

U. S. EPA. 1988b. Guidance on remedial actions for contaminated ground water at Superfund sites. EPA/540/G-88/003, Interim Final.

van der Heijde, P.K.M.. 1987. Quality assurance in computer simulations of ground water contamination. EPA/600/J-87/084, PB-124524. Also pub. in Environmental Software, V.2, n. 1, p. 19-25.

Wilkinson, G.F. and G.E. Runkle. 1986. Quality assurance (QA) plan for the computer software supporting the U.S. Nuclear Regulatory Commission's high-level waste management program. NUREG/CR-4369, U.S. Nuclear Regulatory Commission, Washington, D.C.

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## **C O M M E N T   S H E E T**

**The California Environmental Protection Agency will periodically revise this document to reflect the changing needs of its stakeholders and the evolving science of hydrogeologic characterization. As a user of this document, your comments are important to this ongoing process. Please use this sheet to inform us of any errors, deficiencies or suggested improvements to this document. If you identify an error or deficiency, please suggest how it can be corrected. Attach additional sheets if necessary. Send your comments to:**

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